



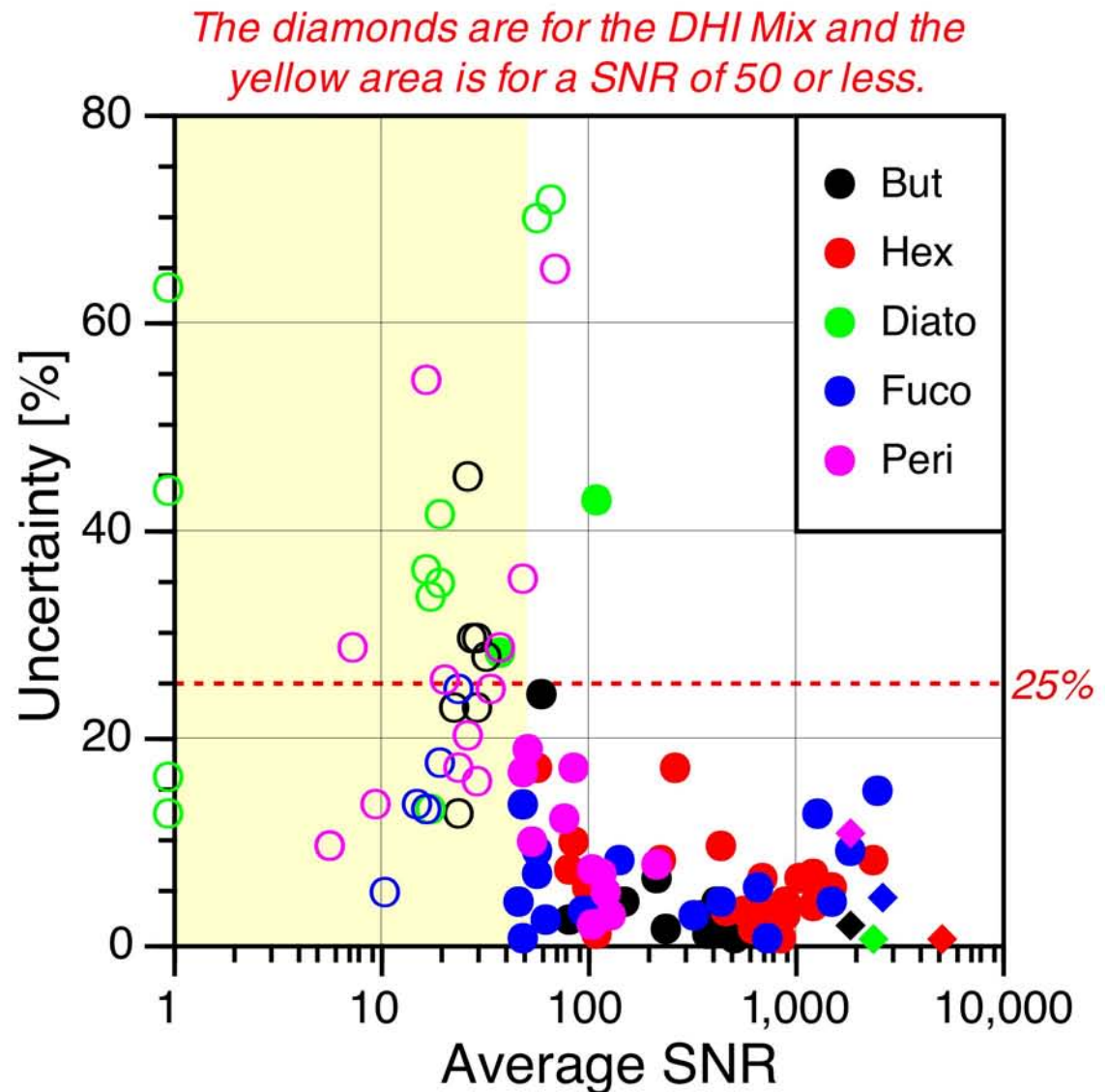
Performance as a Function of Concentration and SNR

Stanford Hooker
NASA/GSFC/CVO
Halethorpe, Maryland



Trace Analyses, Accuracy, and Detectability: *Uncertainties as a Function of SNR*

Individual HPL pigment APDs per sample from SeaHARRE-3 exhibit a strong increase once the SNR is less than 50. A subset of carotenoids, which are frequently found in low concentrations are shown. The data are split into two groups: all QA laboratories agree a pigment is present (solid symbols), and one or more laboratories do not report a pigment as present (open symbols). The data show that when all laboratories do not agree a pigment is present (open circles), the HPL SNR is about 50 or less and the average HPL APDs are 29%; but when all QA laboratories agree a pigment is present (solid symbols), the average HPL APDs are 7%.





The Two-Sentence Rule

The two-sentence rule, seeks to converge reporting strategies without eliminating any data, in particular peaks with low SNRs. The basic objective of the rule is to try and get analysts to do the same thing when they pass through the threshold of reliable quantitation and encounter degraded peak identification caused by problematic absorption spectra.

If a peak is “good” and it can be proved to not be the pigment for that retention time, do not report it; otherwise report it.

If a peak is “bad” and it cannot be disproved to be the correct pigment, report it; otherwise do not report it.

Notice how the burden of proof switches as the quality of the data changes, but in each case the simpler task is accentuated, so analysts will probably be doing less work. When the data is good, the burden is to prove a peak is not going to be correctly identified, and given the good data available, this task will be rather simple. When the data is poor, the burden is to prove the assumption that the peak is correctly identified is in fact false, but because the data are poor, there will be little chance this will be possible, so the usual outcome will be the simple solution of simply reporting it. *Also note the need to agree on what constitutes a good or bad peak.*